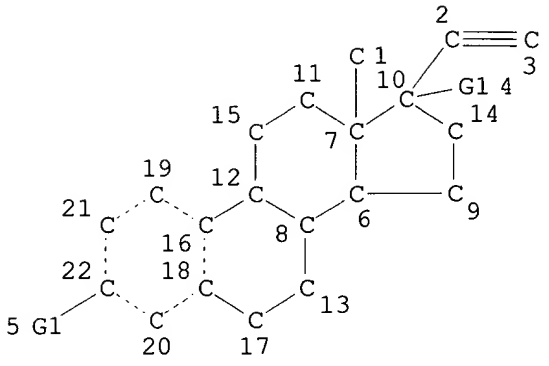
=> d que stat 157
L44 STR



S~Ak
@23 24

VAR G1=23/OH
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L47	649	SEA FILE=REGISTRY SSS FUL L44	
L50	33	SEA FILE=REGISTRY ABB=ON	L47 AND S=1
L52	20	SEA FILE=REGISTRY ABB=ON	L47 AND S>1
L53	53	SEA FILE=REGISTRY ABB=ON	L50 OR L52
L54	48	SEA FILE=REGISTRY ABB=ON	L53 NOT "SULFONYL"
L55	19	SEA FILE=REGISTRY ABB=ON	L54 AND NRS=1
L56	1	SEA FILE=REGISTRY ABB=ON	L55 AND C23H30OS/MF
L57	1	SEA FILE=HCAPLUS ABB=ON	L56

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=> d his 135-159

     (FILE 'HCAPLUS' ENTERED AT 13:25:26 ON 09 OCT 2002)

     FILE 'REGISTRY' ENTERED AT 13:53:51 ON 09 OCT 2002
L35         1308 S 4432.3.65/RID AND NRS=1 AND S=1
L36           12 S L35 AND "ETHYNYL"
L37          119 S 4432.3.65/RID AND NRS=1 AND S>1
L38            0 S L37 AND "ETHYNYL"
L39          110 S 4432.3.65/RID AND NRS=1 AND S=2
L40          119 S L37 OR L39
L41         1427 S L35 OR L37
L42         1285 S L41 NOT "SULFONATE"
L43            4 S L42 AND "ETHYNYL"
L44              STRUCTURE see d que stat L57, attached
L45           39 S L44
L46            7 S L45 AND "ETHYNYL"
L47          649 S L44 FULL
L48           90 S L47 AND "ETHYNYL"
L49            1 S L48 AND "THIO"
L50           33 S L47 AND S=1
L51           29 S L50 NOT "SULFONYL"
L52           20 S L47 AND S>1
L53           53 S L50 OR L52
L54           48 S L53 NOT "SULFONYL"
L55           19 S L54 AND NRS=1 19 compds when narrowed down, but only 1 satisfies
L56            1 S L55 AND C23H30OS/MF <-- "thioether analogs" requirement

     FILE 'HCAPLUS' ENTERED AT 14:50:01 ON 09 OCT 2002
L57            1 S L56 1 cit from CAPlus - attached

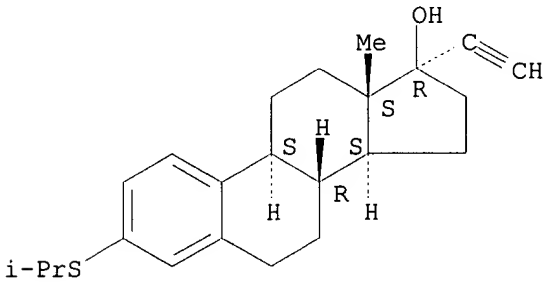
     FILE 'CAOLD' ENTERED AT 14:51:13 ON 09 OCT 2002
L58            0 S L56 0 cits from CAOLD

     FILE 'BEILSTEIN' ENTERED AT 15:23:59 ON 09 OCT 2002
L59            0 S L57 0 cits from Beilstein
```

=> d ibib abs hitstr 1

L57 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:497692 HCAPLUS
DOCUMENT NUMBER: 83:97692
TITLE: Steroids. 14. Sulfur-containing estratrienes
AUTHOR(S): Schwarz, S.; Weber, G.
CORPORATE SOURCE: Wiss. Lab., VEB Jenapharm, Jena, E. Ger.
SOURCE: Pharmazie (1975), 30(5), 277-80
CODEN: PHARAT
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Estrone dimethylthiocarbamate was hydrolyzed by alk. MeOH-H2O to give thioestrone (I) and the disulfide II (RR1 = O). I underwent successive NaBH4 redn., S-alkylation with Me2CHBr, Oppenauer oxidn., and condensation with KC.tplbond.CH to give 3-(isopropylthio)-17-ethynylestra-1,3,5(10)-trien-17.beta.-ol (III). Oxidn. of 3-(isopropylthio)estra-1,3,5(10)-trien-17-one (IV) by excess H2O2 and subsequent condensation with KC.tplbond.CH gave 3-(isopropylsulfonyl)-17-ethynylestra-1,3,5(10)trien-17.beta.-ol (V). The R- and S-isomers of VI were prepd. from IV by oxidn. with 1 equiv. H2O2 and reaction with KC.tplbond.CH, and NaBH4 redn. of I (RR1 = O) gave II (R = HO, R1 = H). III, R-VI, S-VI, and V possessed little or no antigonadotropic activity, but were post-coital contraceptives in rats with their activity decreasing in the order given. III also possessed anticholesteremic activity in rats.
IT **56786-41-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and post-coital contraceptive activity of)
RN 56786-41-5 HCAPLUS
CN 19-Norpregna-1,3,5(10)-trien-20-yn-17-ol, 3-[(1-methylethyl)thio]-, (17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d ibib abs hitstr 1-2

L34 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:247354 HCAPLUS
DOCUMENT NUMBER: 134:261560
TITLE: Therapeutic treatment of androgen receptor driven conditions using steroids or analogs
INVENTOR(S): **Lardy, Henry A.; Marwah, Padma**
PATENT ASSIGNEE(S): Hollis-Eden Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023405	A2	20010405	WO 2000-US26848	20000928
WO 2001023405	A3	20020530		
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000077363	A5	20010430	AU 2000-77363	20000928
EP 1228083	A2	20020807	EP 2000-967114	20000928
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRIORITY APPLN. INFO.:
US 1999-157275P P 19990930
US 1999-157347P P 19990930
US 1999-166116P P 19991116
WO 2000-US26848 W 20000928

OTHER SOURCE(S): MARPAT 134:261560

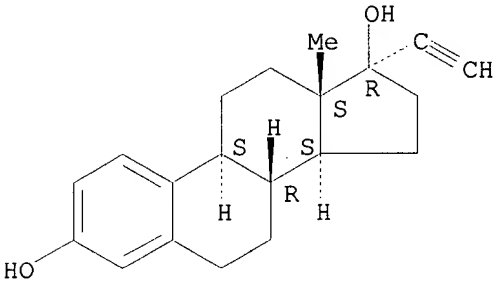
AB A method is claimed to treat or prevent an androgen responsive disease in a subject, or to ameliorate one or more symptoms thereof, comprising administering to a subject, or delivering to the subject's tissues, an effective amt. of a steroid or steroid analogs. The steroid is specifically an analog of 1,3,5(10)-**estratriene**-17.alpha.-**ethynyl**-3.beta.,17.beta.-diol; 17.alpha.-**ethynylandrostene**-3.beta.,17.beta.-diol; 3.beta.,17.beta.-dihydroxyandrost-5-en-16-one; or 3.beta.-methylcarbonate-androst-5-en-7,17-dione. The androgen responsive disease is prostate cancer, benign prostatic hyperplasia, breast cancer, alopecia, acne, hypogonadism or hirsutism. The method further comprises administering to the subject a second therapy; the second therapeutic agent is hydroxyflutamide, leuprolide, megesterol, diethylstilbesterol, aminoglutethimide, spironolactone, tamoxifen, cyproterone acetate, or bicalutamide.

IT **57-63-6DP**, analogs **1159-66-6DP**, 3.beta.,17.beta.-Dihydroxyandrost-5-en-16-one, analogs **3604-60-2DP**, analogs **250163-05-4DP**, analogs
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(therapeutic treatment of androgen receptor driven conditions using steroids or analogs)

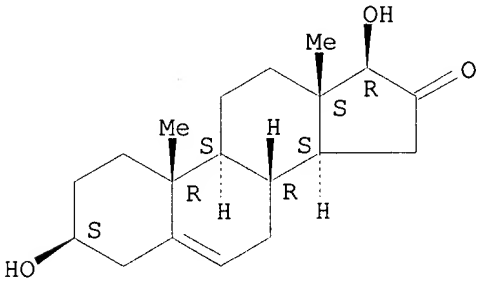
RN 57-63-6 HCAPLUS
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



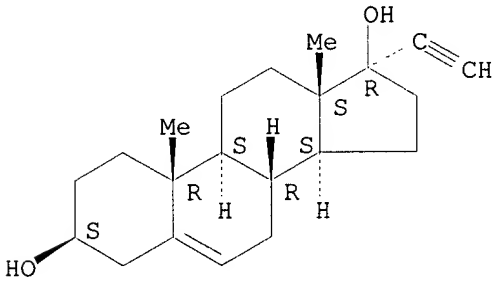
RN 1159-66-6 HCAPLUS
CN Androst-5-en-16-one, 3,17-dihydroxy-, (3.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



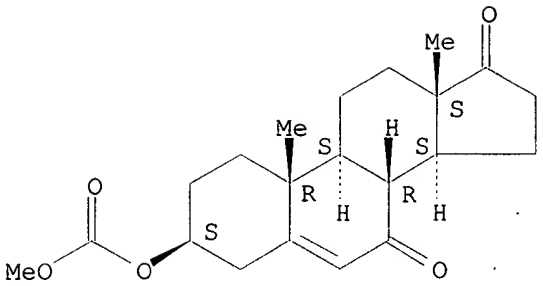
RN 3604-60-2 HCAPLUS
CN Pregn-5-en-20-yne-3,17-diol, (3.beta.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 250163-05-4 HCAPLUS
CN Androst-5-ene-7,17-dione, 3-[(methoxycarbonyl)oxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

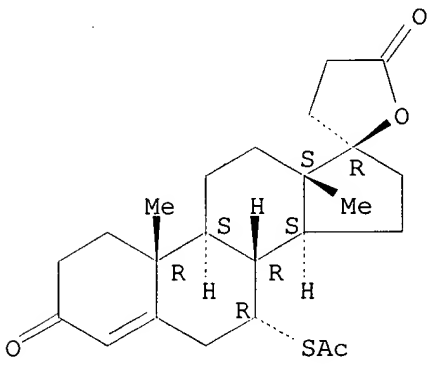
Absolute stereochemistry.



IT **52-01-7**, Spironolactone **56-53-1 125-84-8**,
Aminoglutethimide **427-51-0**, Cyproterone acetate
3562-63-8 10540-29-1, Tamoxifen **52806-53-8**,
Hydroxyflutamide **53714-56-0**, Leuprolide **90357-06-5**,
Bicalutamide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(therapeutic treatment of androgen receptor driven conditions using steroids or analogs in combination with a second therapeutic agent)

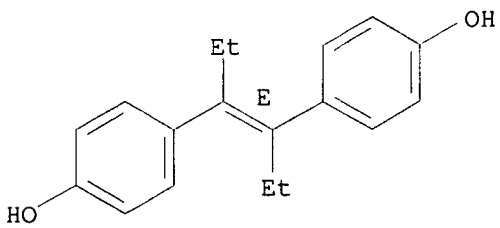
RN 52-01-7 HCAPLUS
CN Pregn-4-ene-21-carboxylic acid, 7-(acetylthio)-17-hydroxy-3-oxo-, .gamma.-lactone, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



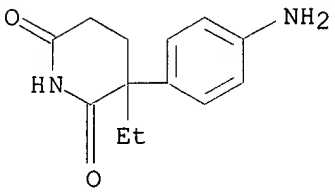
RN 56-53-1 HCAPLUS
CN Phenol, 4,4'-[(1E)-1,2-diethyl-1,2-ethenediyl]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



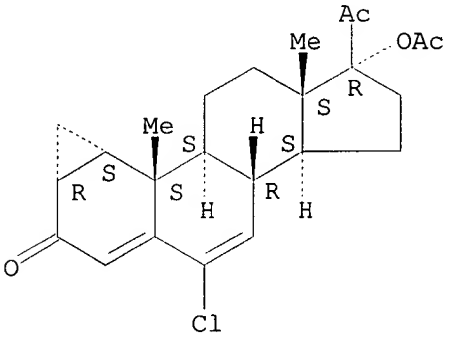
RN 125-84-8 HCAPLUS

CN 2,6-Piperidinedione, 3-(4-aminophenyl)-3-ethyl- (9CI) (CA INDEX NAME)



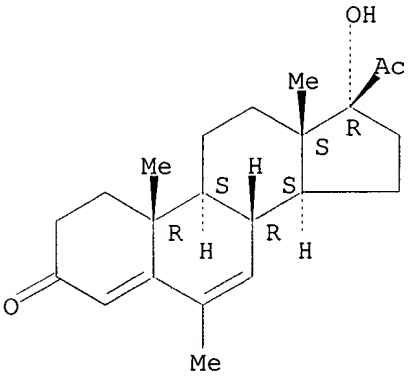
RN 427-51-0 HCAPLUS
CN 3'H-Cyclopropa[1,2]pregna-1,4,6-triene-3,20-dione, 17-(acetyloxy)-6-chloro-1,2-dihydro-, (1.beta.,2.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



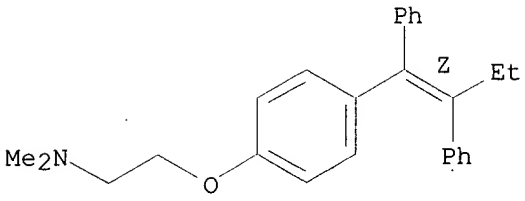
RN 3562-63-8 HCAPLUS
CN Pregna-4,6-diene-3,20-dione, 17-hydroxy-6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

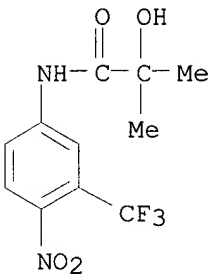


RN 10540-29-1 HCAPLUS
CN Ethanamine, 2-[4-[(1Z)-1,2-diphenyl-1-butenyl]phenoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



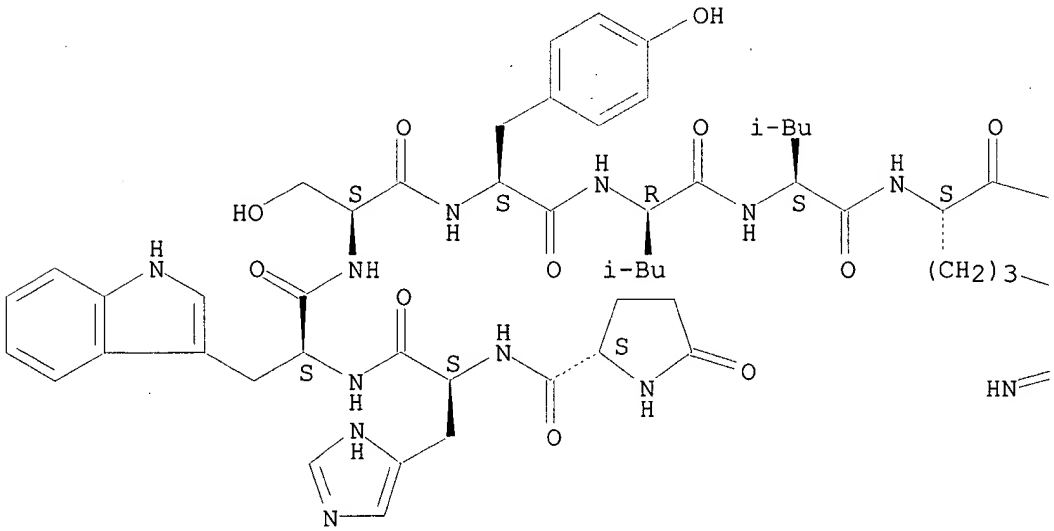
RN 52806-53-8 HCAPLUS
CN Propanamide, 2-hydroxy-2-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

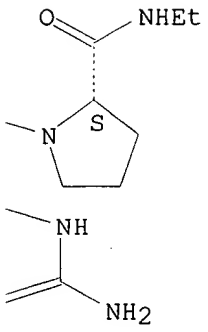


RN 53714-56-0 HCAPLUS
CN 1-9-Luteinizing hormone-releasing factor (swine), 6-D-leucine-9-(N-ethyl-L-prolinamide)- (9CI) (CA INDEX NAME)

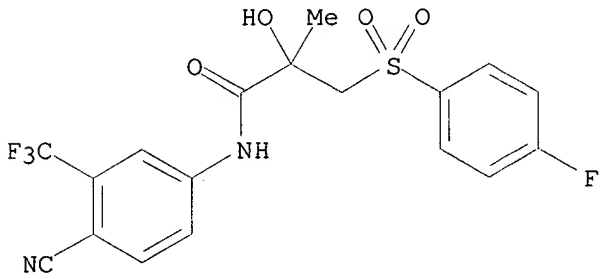
Absolute stereochemistry. Rotation (-).

PAGE 1-A





RN 90357-06-5 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

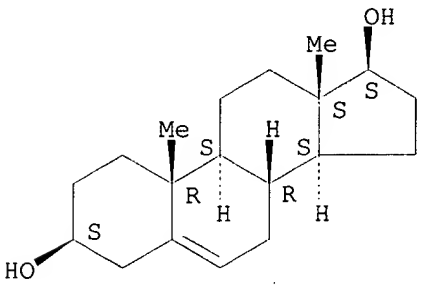
L34 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:684497 HCAPLUS
DOCUMENT NUMBER: 131:332293
TITLE: Suppression of .DELTA.5-androstenediol-induced androgen receptor transactivation by selective steroids in human prostate cancer cells
AUTHOR(S): Chang, Hong-Chiang; Miyamoto, Hiroshi; **Marwah, Padma**; **Lardy, Henry**; Yeh, Shuyuan; Huang, Ko-En; Chang, Chawnshang
CORPORATE SOURCE: George Whipple Laboratory for Cancer Research, Departments of Pathology, Urology, Radiation Oncology, and the Cancer Center, University of Rochester Medical Center, Rochester, NY, 14642, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1999), 96(20), 11173-11177
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors' earlier report suggested that androst-5-ene-3.beta.,7.beta.-diol (.DELTA.5-androstenediol or Adiol) is a natural hormone with

androgenic activity and that two potent anti-androgens, hydroxyflutamide (Eulexin) and bicalutamide (Casodex), fail to block completely the Adiol-induced androgen receptor (AR) transactivation in prostate cancer cells. Here, the authors report the development of a reporter assay to screen several selective steroids with anti-Adiol activity. Among 22 derivs./metabolites of dehydroepiandrosterone, the authors found 4 steroids [no. 4, 1,3,5(10)-**estratriene**-17.alpha.-**ethynyl**-3,17.beta.-diol; no. 6, 17.alpha.-**ethynyl**-androstene-diol; no. 8, 3.beta.,17.beta.-dihydroxy-androst-5-ene-16-one; and no. 10, 3.beta.-methylcarbonate-androst-5-ene-7,17-dione] that have no androgenic activity and could also block the Adiol-induced AR transactivation in prostate cancer PC-3 cells. Interestingly, these compds., in combination with hydroxyflutamide, further suppressed the Adiol-induced AR transactivation. Reporter assays further showed that these four anti-Adiol steroids have relatively lower glucocorticoid, progesterone, and estrogenic activity. Together, these data suggest some selective steroids might have anti-Adiol activity, which may have potential clin. application in the battle against the androgen-dependent prostate cancer growth.

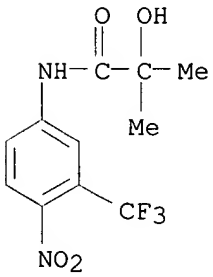
IT **521-17-5**, .DELTA.5-Androstenediol **52806-53-8**, Hydroxyflutamide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(androstenediol-induced androgen receptor transactivation suppression by selective steroids in human prostate cancer cells)

RN 521-17-5 HCAPLUS
CN Androst-5-ene-3,17-diol, (3.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 52806-53-8 HCAPLUS
CN Propanamide, 2-hydroxy-2-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

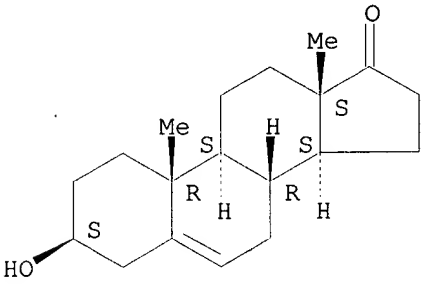


IT **53-43-0D**, Dehydroepiandrosterone, metabolites **57-63-6**

1159-66-6 3604-60-2 250163-05-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(androstenediol-induced androgen receptor transactivation suppression by selective steroids in human prostate cancer cells)

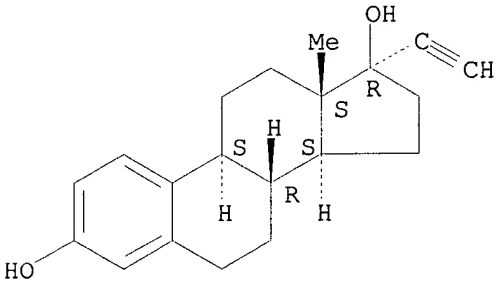
RN 53-43-0 HCAPLUS
CN Androst-5-en-17-one, 3-hydroxy-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



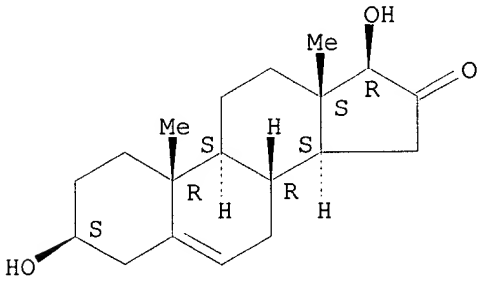
RN 57-63-6 HCAPLUS
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 1159-66-6 HCAPLUS
CN Androst-5-en-16-one, 3,17-dihydroxy-, (3.beta.,17.beta.)- (9CI) (CA INDEX NAME)

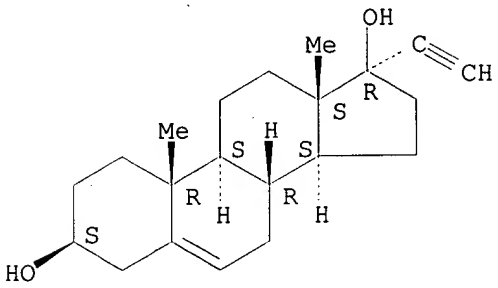
Absolute stereochemistry.



RN 3604-60-2 HCAPLUS

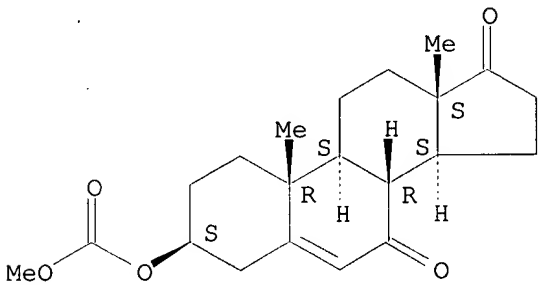
CN Pregn-5-en-20-yne-3,17-diol, (3.beta.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



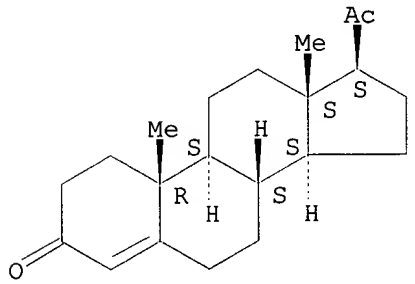
RN 250163-05-4 HCAPLUS
CN Androst-5-ene-7,17-dione, 3-[(methoxycarbonyl)oxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **57-83-0**, Progesterone, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(androstenediol-induced androgen receptor transactivation suppression by selective steroids in human prostate cancer cells)
RN 57-83-0 HCAPLUS
CN Pregn-4-ene-3,20-dione (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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